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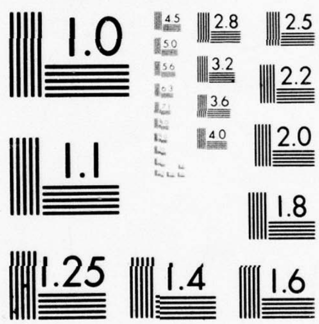

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EXTENDED NEUTRAL WIND MODELLING

Physical Dynamics, Inc.
P.O. Box 1069
Berkeley, California 94701

June 1977

Topical Report for Period November 1975—June 1977

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The application of acoustic gravity wave mechanics to modelling neutral winds in the high altitude nuclear environment is discussed. Particular emphasis is placed on the problem of late time and large distance from the burst center. Specific work on coupling modes to hydro code output is reported. A technique to greatly extend the boundaries in scenario studies is also reported.

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I. INTRODUCTION

It is well established that cross-field flows of neutral wind govern the physics of plasma structure in the high-altitude nuclear environment.[1] The description of this wind is, obviously, a central issue in constructing numerical simulations of the plasma phenomenology. In many cases, limitations have arisen in previous research and systems analysis efforts because of the lack of a suitable routine to predict these flows.[2] The development of a procedure to correct this deficiency is the subject of this document. The work is specifically directed at constructing a driver for electrostatic ion motion codes in the late-time communication regime. Oriented towards this particular purpose, the program has a two-fold objective. First, it focuses on our desire to extend the ability to calculate to very late times (hours) and to very great distances (thousands of kilometers). Second, it emphasizes the development of quick running, flexible procedures for application in arbitrary scenarios.

The flow modelling is based on the superposition of acoustic gravity wave (AGW) modes. The heart of the computational work is a comprehensive, three-dimensional (32×32×32) AGW simulator developed in a previous contractual effort. The relevant AGW mechanics and technical details

of the code have been thoroughly described in DNA 3420T[3] and will not be repeated here. Our purpose in this document is to review the further application of this technique to several new facets of the modelling effort which have been undertaken in the current year. It does seem appropriate at this point, however, to quickly review the rationale for selecting an AGW approach to the general problem of modelling an extended space/time neutral wind.

Following a nuclear event, the atmosphere is set into motion by pressure enhancements which arise either directly at a burst or at distant locations due to radiation deposition. For large bursts at high altitude, the resulting motion is strongly influenced by the Earth's gravity, both directly and through the stratified ambient density. The atmosphere is an acoustic-gravitational medium which relieves these nonequilibrium pressures by sending out pulses which set the fluid in motion. A natural representation of the response is in terms of a set of acoustic-gravity waves. In general, the solution of the fully nonlinear fluid equations using the AGW approach is a complex undertaking. In fact, prior to the advent of Fast Fourier Transform (FFT) techniques, one would not choose to go this route except in very special circumstances. Thus, it has become customary to solve nuclear event hydrodynamic

problems using finite differencing in physical space of the familiar fluid equations. This differencing is arbitrary and, perhaps, to a mathematician "unnatural", but has been the only real avenue open for obtaining practical results. The introduction of the FFT has changed the traditional odds markedly. Today it can be argued that the solution of fluid problems in appropriate wave-number space is no more complex than the older techniques and stands to give better answers. Nonetheless, we would not be prepared to make the case that a complete AGW code could improve on MRHYDE or MICE without extensive and costly development. It is important to keep this last statement in mind. There is <u>no</u> suggestion in this paper that present general hydro codes are obsolete or ought to be replaced. The discussion is concerned with augmenting the utility of these codes by adding to our capability in an extended space/time regime.

When we shift our attention from the early-time/close-in regime to the late-time/far-distance regime, the equations that govern the neutral background flows take on an increasing linear character. It is, as we approach this regime, that present hydro codes begin to experience serious difficulties. It can be argued that the very characteristics which enabled them to do an excellent job at the start of

the calculation are now causing them trouble. The inclusion of all the nonlinear terms is amplifying noise to the point of unreliability. The finite difference mesh forces intolerably small time steps. What is clearly needed is a simpler reformulation of the problem which can permit extension into the new regime.

In the truly linear regime, such as the ambient atmosphere, there can be little argument but that flow problems ought to be formulated in terms of AGW. The technique has been highly developed and is universally used in research concerning travelling ionospheric disturbances and other high-altitude neutral phenomena. The popularity of the procedure is based on the issue of "natural" representation. If the medium can be approximated as linear, then we can express a disturbance as a set of acoustic gravity waves whose frequency and amplitude are <u>constants</u>. It becomes a simple matter to reconstruct the evolving disturbance at any arbitrary subsequent time or place by a simple superposition of these waves. Utilizing the FFT to perform the initial wave analysis and subsequent reconstructions, we have a procedure that is quick, convenient, and reliable. In the linear regime, the identification and preservation of the constants of the wave structures assures fidelity and absence of numerical noise.

The ability to superpose uncouples us from artificial constraints related to grid-size/time-step requirements.

It seems obvious to us that a complete cycle for the neutral flow calculation ought to begin with the familiar hydro code at early time and end with an AGW code at late time. Now if we are to marry the early time and the late time, there must be a common meeting ground established with a comfortable overlap. Having commented on the problems of nonlinear, finite difference hydro codes in going to late time, it is appropriate to comment on what happens to an AGW code when it goes to early time. If we formulate our fluid dynamics as a set of acoustic gravity waves and monitor their behavior in the highly nonlinear regime, we will observe that their amplitude and frequency are <u>not</u> constants, but vary with time. Expressed more precisely, we will find that the evolution of a disturbance does not retain a fixed modal representation that can arbitrarily be reconstructed by superposition of the initial waves. Instead we find a continuous transfer of energy from one set of modes to another, which alters the respective amplitudes. Simultaneously, because the modes are interactive, the frequency is shifted from its "natural" value. The calculation of these amplitude and frequency changes would be the heart

of a fully coupled AGW code. As implied before, we have not constructed such a code, but would expect it to be equal in complexity to the traditional codes.

The basic plan to marry a "constant coefficient" AGW code to a general hydro code run is, perhaps, obvious at this point. We need to monitor the AGW parameters in the hydro code run to determine when they have settled down and appear to be approaching constant values. Clearly, they will never be exactly constant. It will be necessary to employ some engineering criterion with respect to statements such as "sufficiently constant". The next section of this review is devoted to the subject of interfacing an AGW solution to the end point of a MICE hydro code run.[4]

Strictly from a physics veiwpoint, the main task in utilizing constant coefficient AGW mechanics for neutral wind modelling is solely the question of coupling to a suitable set of initial conditions. In a multiburst scenario, there is the need to stop and restart with new coefficients for each new burst. However, this is really just a computational detail that was reasonably well explored in previous work (DNA 3420T).[3] Essentially, if one can couple to a single burst, it should be possible to also couple to repeated bursts at later times or different locations with

similar procedures. If we were using a Fourier Integral of infinite (or Earth circumference) dimension, there would be no additional computational task in the development program. As it is, we employ Fourier Transforms of distinctly finite spatial extent and, in particular, use fast Fourier procedures. While we have, from time to time, looked into alternative numerical techniques, we have always returned to the position that the use of the FFT is an essential ingredient. It is the FFT which permits extremely short running time and reliable manipulation of massive blocks of physical and Fourier data.

The use of FFT procedures introduces a potential limitation on the maximum size of our spatial grid. As our objective is to extend the flow solution to the large space/time regime, it is our desire to minimize any restriction of this type. Consequently, a significant effort has been made to develop auxiliary procedures to overcome this problem with the FFT. We believe that the current research program has been successful in generating a solution to this difficulty. The third section of this document is devoted to a discussion of this issue.

We can summarize the rationale and features of the overall program as follows. First, an extended space/time neutral wind model is a requirement of the plasma phenomenology

that is relevant to communication systems analysis. Second, a formulation based on AGW mechanics is the logical approach to model construction. Third, a basic AGW simulation has been built and tested in earlier work. Fourth, in application there are two development problems: (A) coupling to a hydro code, and (B) overcoming any grid limitations imposed by the use of FFT.

II. HYDRO CODE COUPLING

In order to initiate a legitimate high-altitude nuclear calculation using the constant coefficient AGW procedure, it has appeared desirable to start from hydro code data as indicated in the last section. Ultimately, for use in broad ranging scenario studies, it would seem desirable to construct a family of "initializers". These would constitute a library of simpler data sets that would give equivalent flow properties for starting not only an extended wind model, but also a variety of concurrent late-time plasma modelling schemes. Sowle of Mission Research Corporation has proposed such an activity, and we strongly support the idea.[5] In the meantime, the employment of actual hydro code data tapes appears to be the easiest way to both start AGW computations and to insert mode corrections in simulating multiburst flows.

The input and manipulation of hydro code data for use in extended space/time wind studies is conceptually straightforward, but non-trivial in practice. Fajen and co-workers at MRC have been most cooperative in making the library of MICE tapes available to us and providing instructions on reading and storing the data.[4] With their assistance, we have become proficient in using the data. As a prototype run for use in developing procedures, we

have focused on the S200 data with vertical magnetic field. This case possesses two important features: 1) it is the "canonical" high-altitude burst, and 2) it is expected to display very large nonlinear effects at early time. In understanding the behavior of this run, we have assumed that we were observing characteristics that would be typical of all such data sets.

The major nonlinear effect in high-altitude bursts is the rapid vertical rise of fluid in columns near the fireball core. Because the neutral fluid is partially coupled to the plasma in the core (which is in turn tied to the field), this effect is maximized in a vertical field geometry. The altitude regime of primary interest to us is the space form 125 km to 500 km. The S200 is of a size and location to produce a large effect in this range.

The first step in building an interface between hydro code data and the AGW procedure is to investigate the behavior of the early-time data in terms of its acoustic gravity wave properties. We can accomplish this task by computing the actual mode amplitude of each AGW as a function of time. Each mode is identified by a complex amplitude which we can write as

$$A = R\, e^{i\theta} \qquad (1)$$

where R is a real modulus and θ is a real phase angle. We can describe the phase variation in time by defining a real frequency, Ω,

$$\theta = \theta_o + \Omega t \quad . \tag{2}$$

In the linear regime, we would select R and θ_o as initial constants. Ω would be a constant frequency for the particular mode determined by a dispersion relation. We would determine the value of A at any subsequent time by merely consulting these constants. In the nonlinear regime, however, we can expect R to vary in time and the value of θ will not be given exactly by (2). Thus, our specific task is to find the actual values of R that MICE is generating and, likewise, the actual values of θ. With respect to the latter, it is convenient to remove the natural phase rotation and consider only the phase difference as a function of time.

$$\phi = \Delta\theta = \theta - \Omega t \tag{3}$$

The algebraic steps in constructing a set of complex amplitudes, A, from an arbitrary data set is straightforward but tedious. It has been explained in detail in DNA 3420T[3] and will not be repeated here.

As a general proposition, we can resolve the MICE flow field into an arbitrarily large number of AGW modes. As a practical matter, it would not make sense to consider modes with characteristic dimensions less than the MICE spatial resolution. Such modes would prove to have negligible amplitude and their consideration would be wasteful of our computer storage capability. We have found that there is no difficulty in fitting the MICE output if we confine ourselves to modes whose quarter-cycle dimension is greater than 45 km.

The other side of the coin concerns the size of the maximum dimension to consider in the problem. To follow the evolution of the hydrodynamics for extended periods in time, the spatial dimensions can become enormous. Our ultimate objective is to be able to work in a space that is 12,000 km in extent. The techniques for computing in such a vast spatial domain require special development and form the subject of the next section of this document. For the immediate purpose of investigating the MICE data, however, we have not employed these procedures, nor are they necessary. In the relatively early time frame for which MICE computes output, we find that spatial dimensions of 3000 km horizontal and 1700 km vertical are adequate. We therefore limit the resolution into AGW modes whose half-cycle dimension is less than these values.

Bounded by the limits discussed above, our basic AGW simulation will construct amplitude parameters for 131,072 modes. The S200 run displays spatial data from zero to about 550 seconds at approximately 30 distinct time steps. Our task has been to construct the amplitude parameters for each mode at each time step and plot the results. For each mode, we have computed the time-dependent value of R and ϕ. This result is, obviously, 262,144 separate curves. These have been computer plotted and stored on microfiche. Both parameters are displayed in a common space with banks of six modes fitted on a fiche grid, as shown in Figure 1. With this compression, we can fit about 50,000 plots on a single fiche.

While the AGW data set for the MICE S200 run may sound overwhelmingly large, it is actually simpler to view and comprehend than many displays we have seen of the physical flow-field data. Because all of the curves are essentially similar, it was possible to survey a vast array simultaneously and deduce the information that we were looking for.

Figure 1 is a convenient example to employ in describing the analysis of AGW behavior. It happens to contain the largest amplitude modes and thus was the most important single data set. It displays the characteristic time

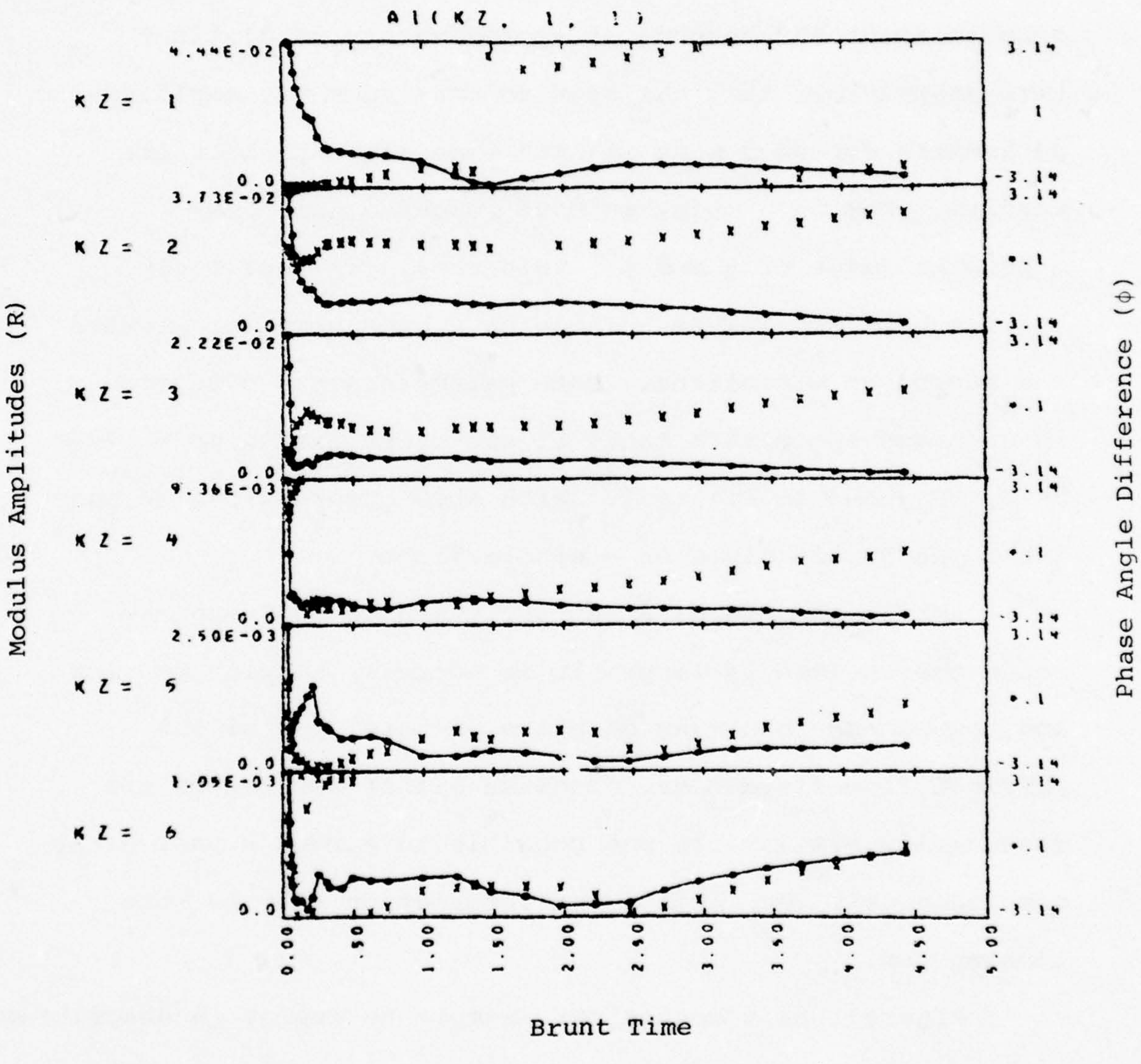

Figure 1. S200 MICE AGW amplitudes.

of "numerical noise" in MICE, which is not real and should be ignored. In any event, there is the possibility that much of this drifting will cancel out when the modes are summed up to obtain true physical representations.

Ideally, we would always like to couple the constant coefficient AGW solution to a hydro code run at a point in time when we were absolutely certain that R and ϕ were stationary. We could then extend the solution as far as we wished, knowing that our numerical simulation was "exact". Our study of MICE S200 has demonstrated, however, that we are not likely to be given such data. Undoubtedly, we will also have to start when these parameters are still drifting, the "quasi-linear regime". The question will then arise as to the "legitimacy" of coupling at this point. Obviously, we cannot provide a definitive answer by simply analyzing mode amplitude data. The latter is highly useful for defining regimes and indicating possibilities. It is not clear, though, that it provides a simple quantitative assessment of the influence of parameter deviations on the ultimate physical solution.

The basic objective of the extended neutral wind program is to provide cross-field wind velocities and neutral densities for use by plasma phenomenology routines. In the end, the program will be judged on the reliability

of these results and not on the stationarity of AGW mode parameters. It has seemed, therefore, that a valuable exercise would be to compare a constant coefficient simulation in the quasi-linear regime to the MICE simulation. The time interval from 300 to 450 seconds appears to be an appropriate span to consider. As indicated in the discussion above, we believe that the AGW mode analysis is telling us that this is not an unreasonable choice. Prior to 300 seconds, the S200 appears to show mode coupling. After 450 seconds, we observe boundary problems in the MICE grid that are irrelevant to the real physics that we wish to simulate.

In Figure 2, we show contour plots of the logarithm of the density perturbation from the MRC MICE S200 at 300 seconds. The vertical dimension is altitude in units of 200 km. The top boundary is 1200 km. The "X" dimension of our 3-D code is equivalent to their radius in the same units as above. The radial boundary is 1050 km. We are going to analyze the MRC data at this time frame into AGW modes. For two reasons, we do not want their large perturbation quantities up against the boundary of our grid. We desire to provide a reservoir region surrounding the data to avoid artificial steep gradients in the AGW resolution. We also want to provide space for the solution

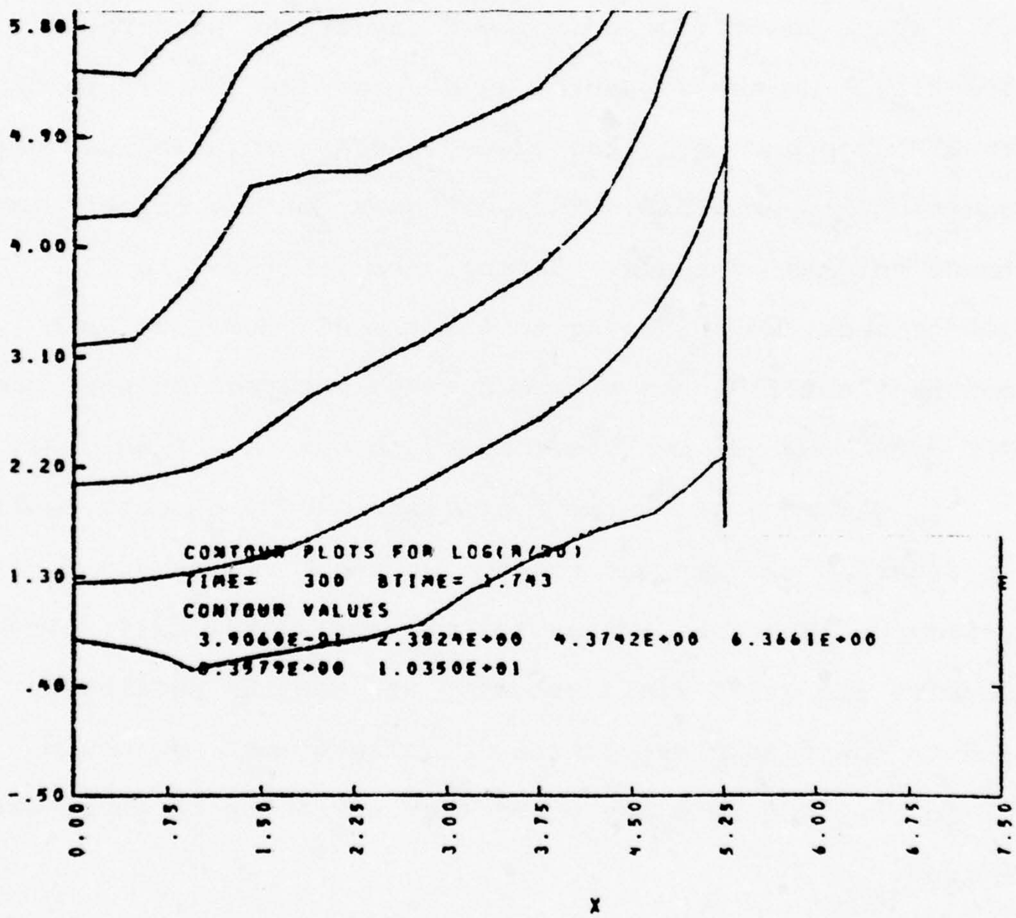

Figure 2. MRC density - 300 seconds.

to evolve without hitting the boundary. To accomplish this, we establish a vertical space from -50 to +1750 km and a horizontal space from -1500 to +1500 km.

In Figure 3, we show the extension of MRC data into this space to provide a smooth decay of the perturbed quantity. On the same plot we display the AGW fit to MRC at 300 seconds. Near the edges, the AGW solution has been additionally smoothed. Thus, it does not fit exactly in these volumes of space. Having once fit the data at 300 seconds, we are going to let the AGW code run with constant coefficients and no further interaction with the MRC data. We can run the comparison out to 450 seconds.

Figure 4 shows the comparison at 330 seconds, while in Figure 5 we jump out to 450 seconds. Figures 6, 7, and 8 provide the same display for the radial velocity. The density and cross-field velocity are the two parameters fed to the plasma electrostatic integration. We could, of course, generate any other flow parameter if there was a need.

It is important to emphasize that the figures show both the battle space <u>and</u> the reservoir. The reservoir is <u>garbage</u> for purposes of this comparison. One should review Figure 2 to observe the actual MICE grid space which would be equivalent to the battle space. We believe that the

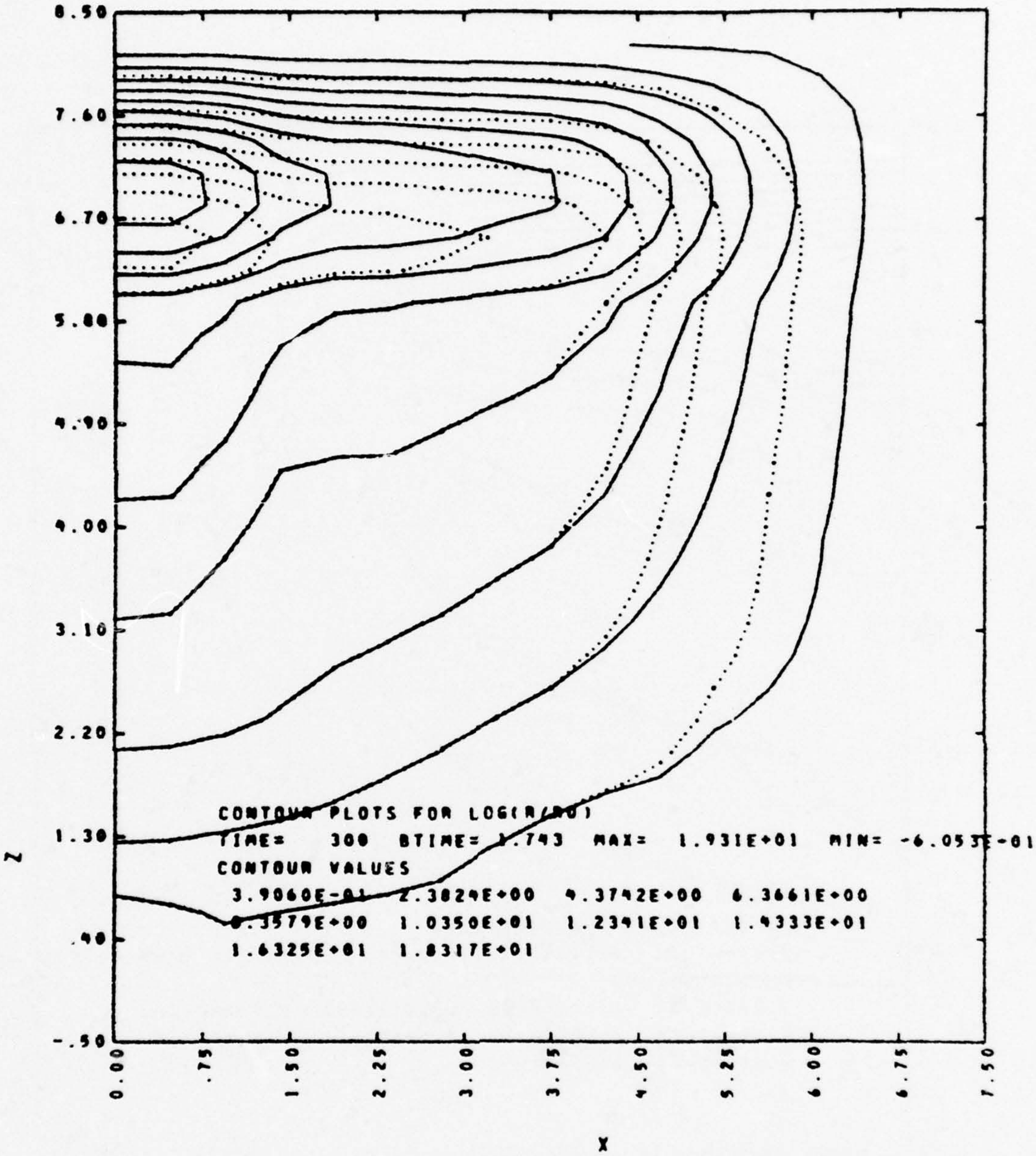

Figure 3. Comparative density - 300 seconds

———————————— = MICE

------------ = AGW

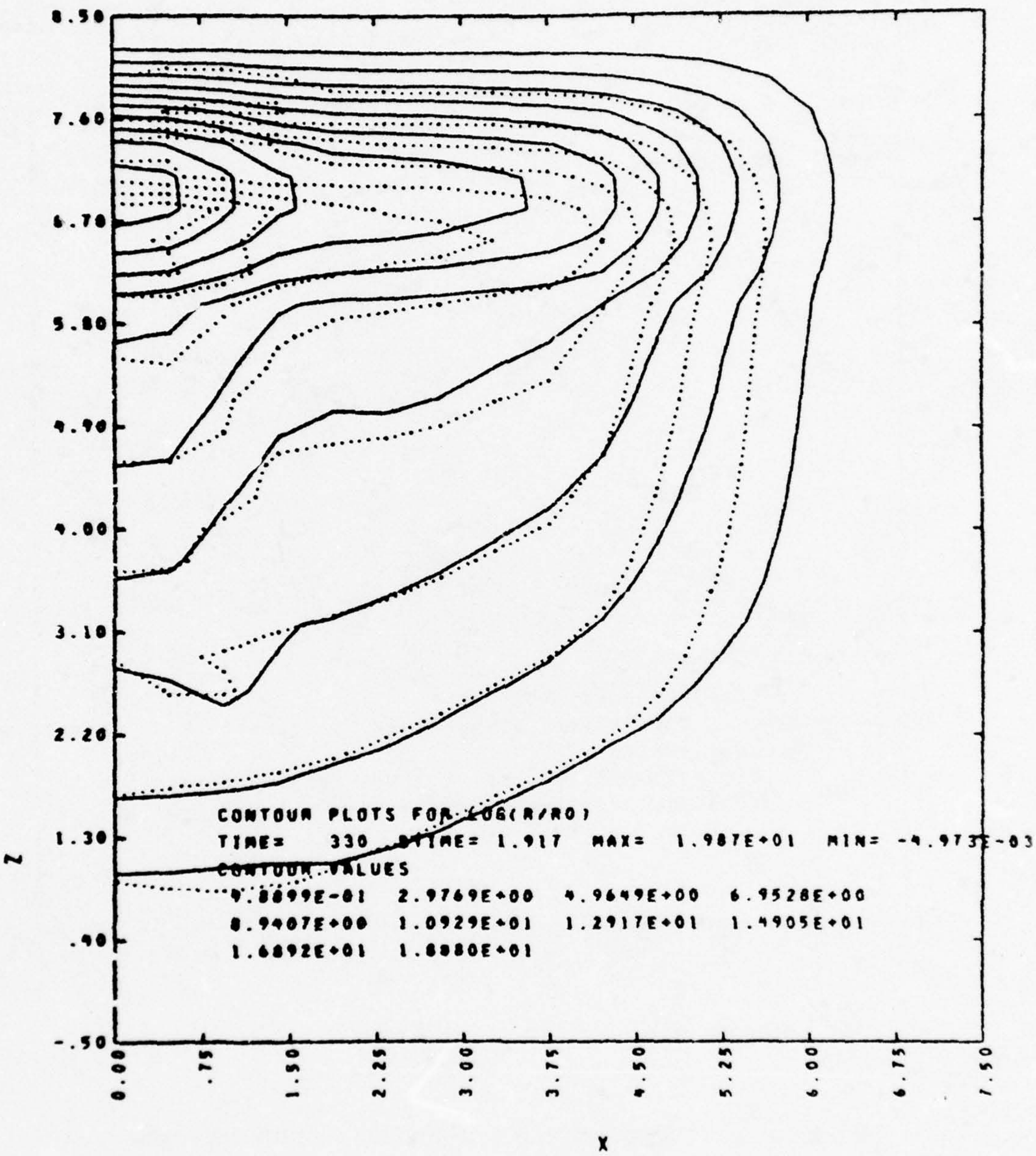

Figure 4. Comparative density - 330 seconds.

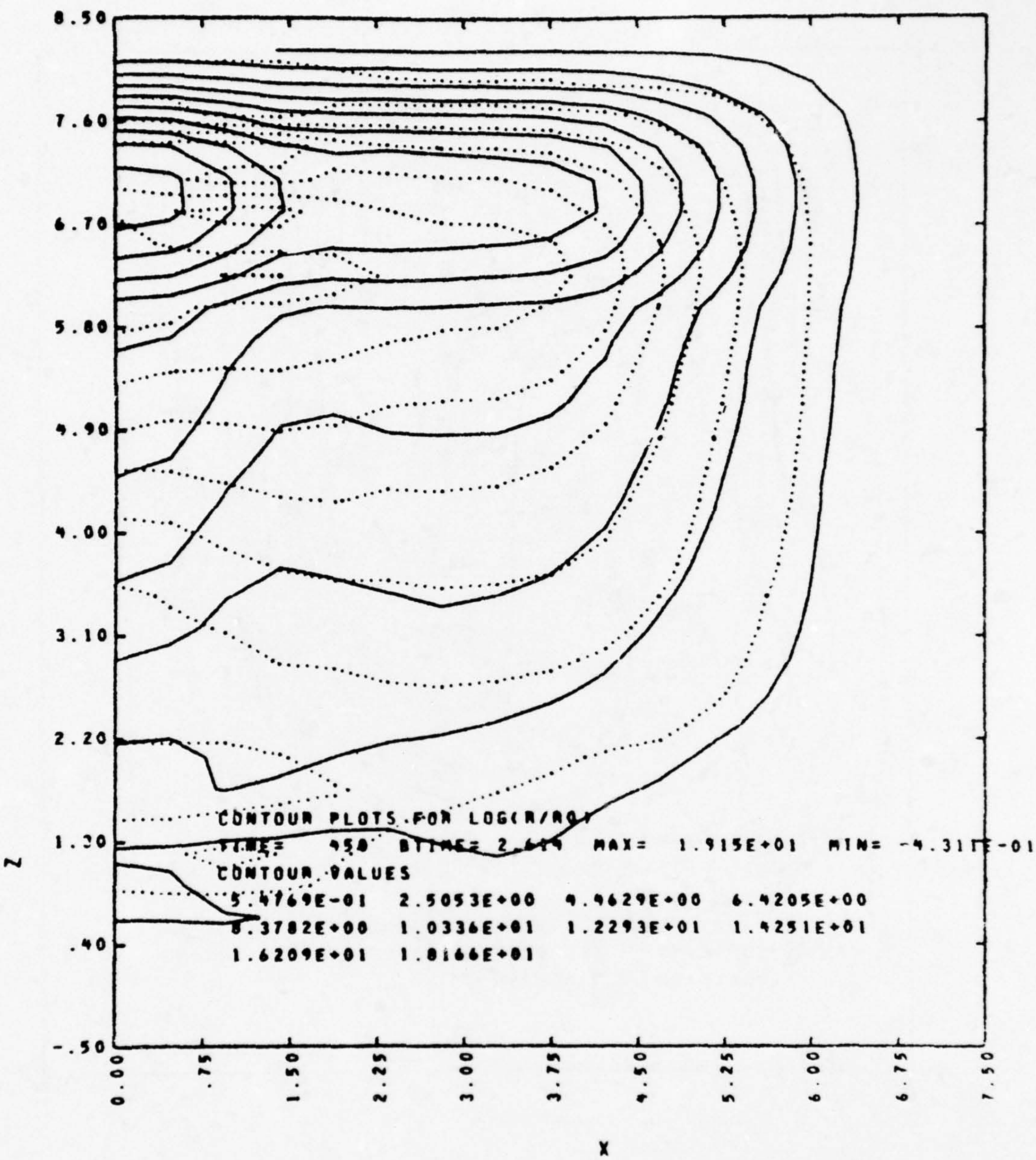

Figure 5. Comparative density - 450 seconds.

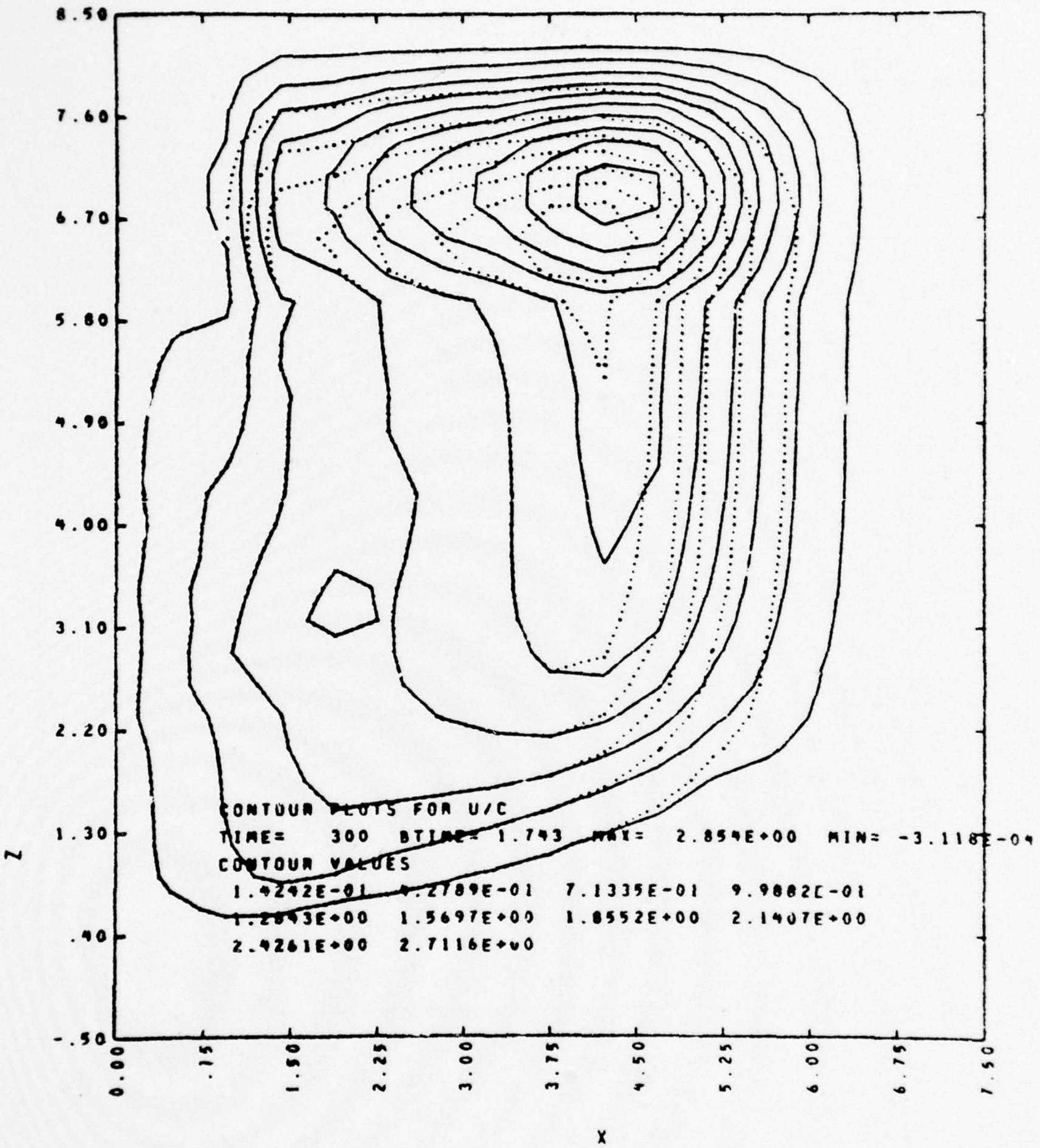

Figure 6. Comparative radial velocity - 300 seconds.

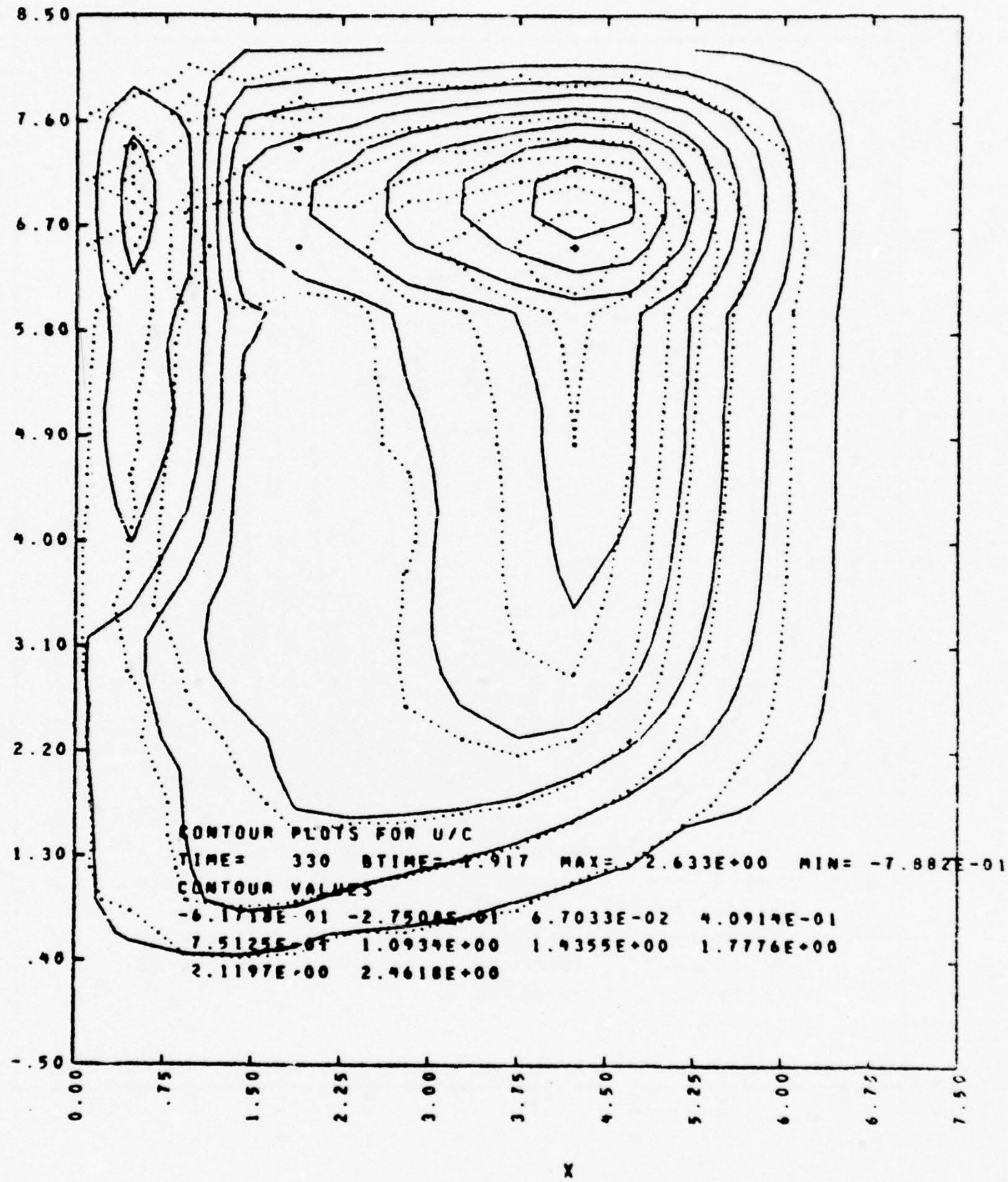

Figure 7. Comparative radial velocity - 330 seconds.

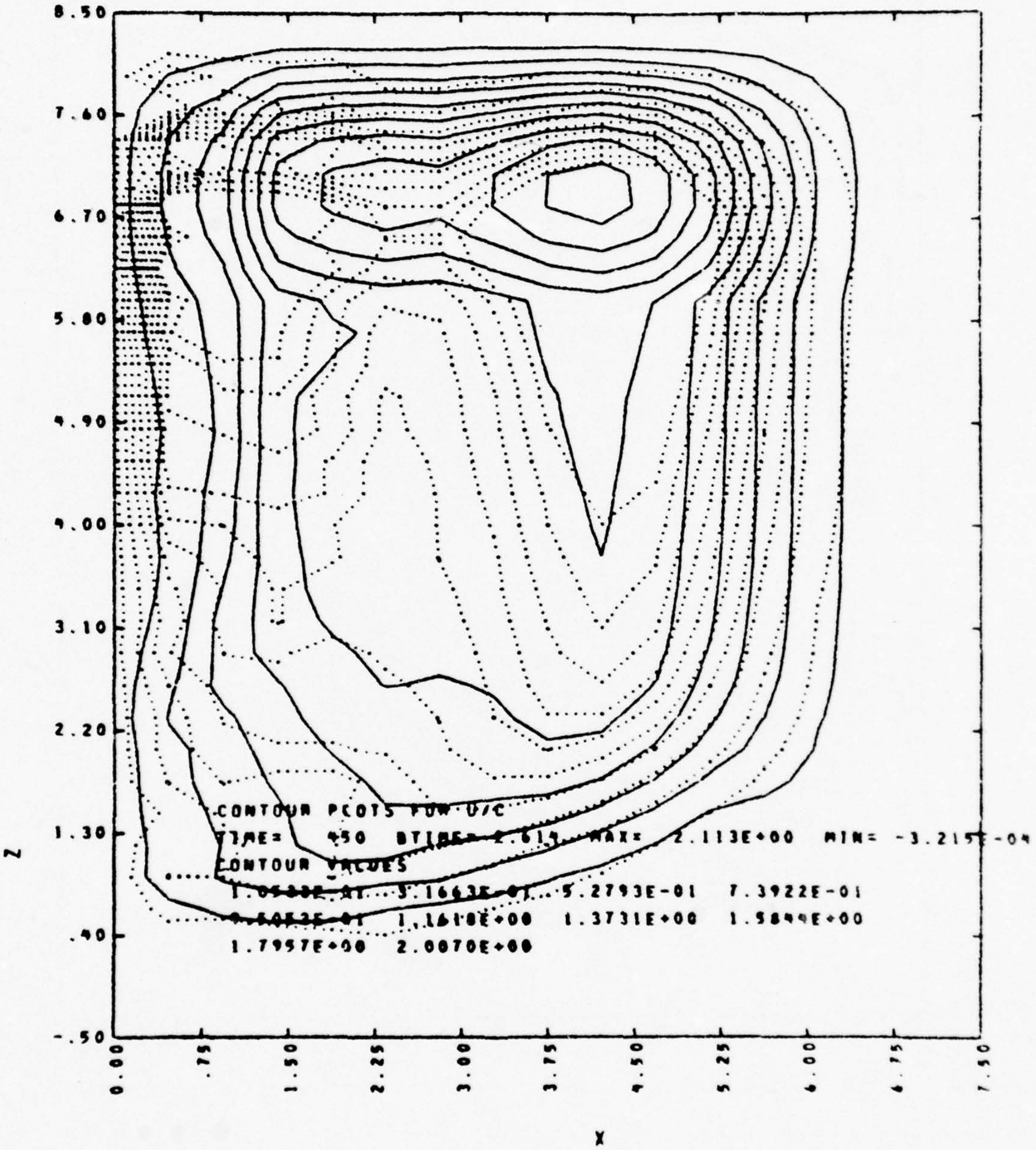

Figure 8. Comparative radial velocity - 450 seconds.

comparison in the battle space region is quite encouraging.

We do note that there are problems in getting a good comparison along the central axis core. The AGW solution has a tendency to overemphasize the central ballistic rise of fluid. (It is well known that "linear" procedures overestimate effects in the nonlinear regime because of the lack of the convective derivative, which typically provides a saturation or damping influence.) We find the density contours a little higher in this space, while the radial velocity contours are distorted by the upsweep of fluid. We have made no attempt to "tune" our simulation to fit the MICE data. We could probably juggle the gas properties or ambient atmosphere to correct some of the central core discrepancy. We do not believe that this would represent the proper spirit of the simulation, however.

Away from the center line, the flow properties are reasonably well simulated. This is, after all, the major region for striation development and represents, by far, the greatest volume (which may not be obvious in a 2-D plot).

Having coupled to the MICE run and computed the AGW parameters, we can, of course, run the solution out in time. Figure 9-14 show the extension to 2400 seconds. In this

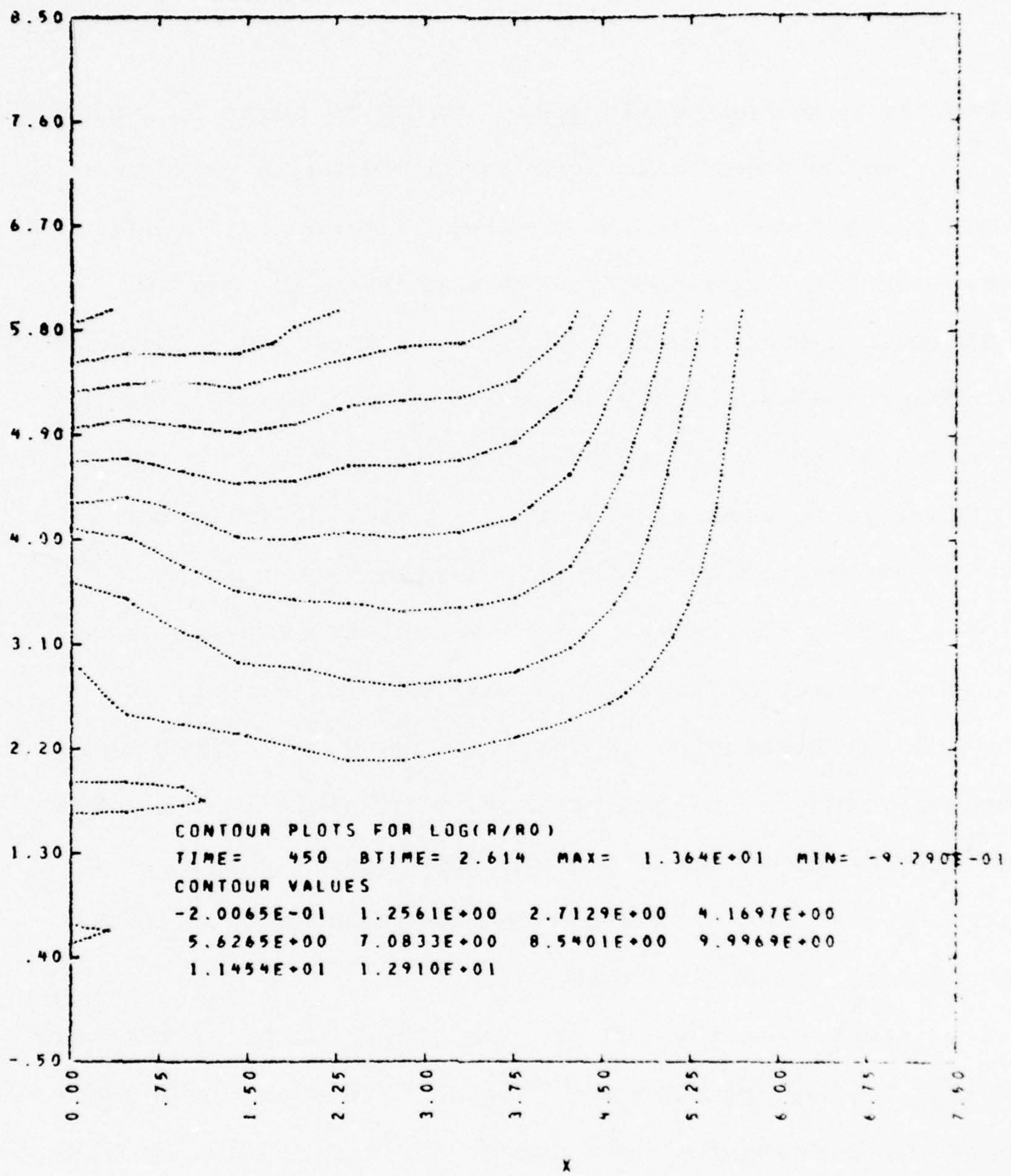

Figure 9. AGW density - 450 seconds.

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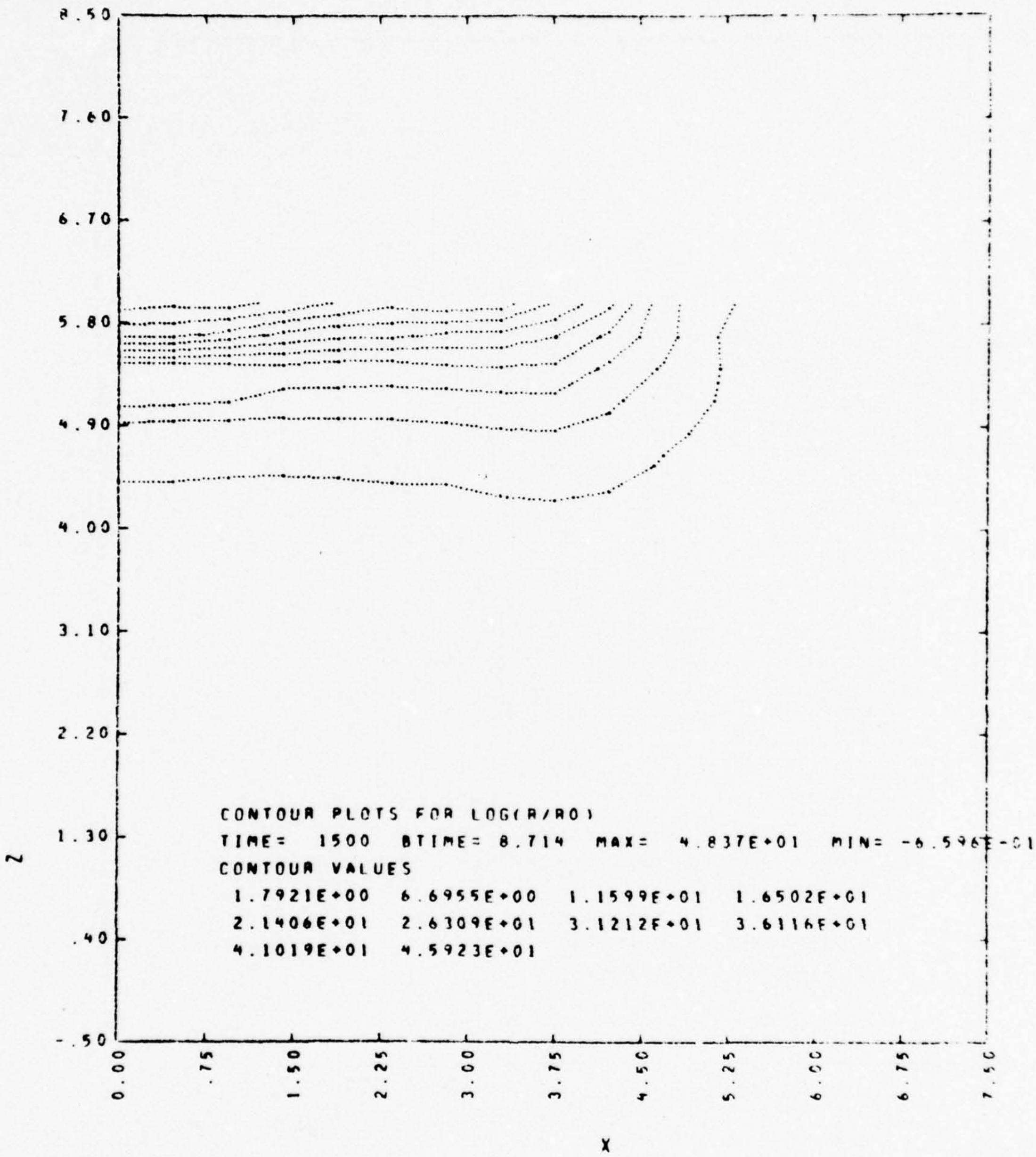

Figure 10. AGW density - 1500 seconds.

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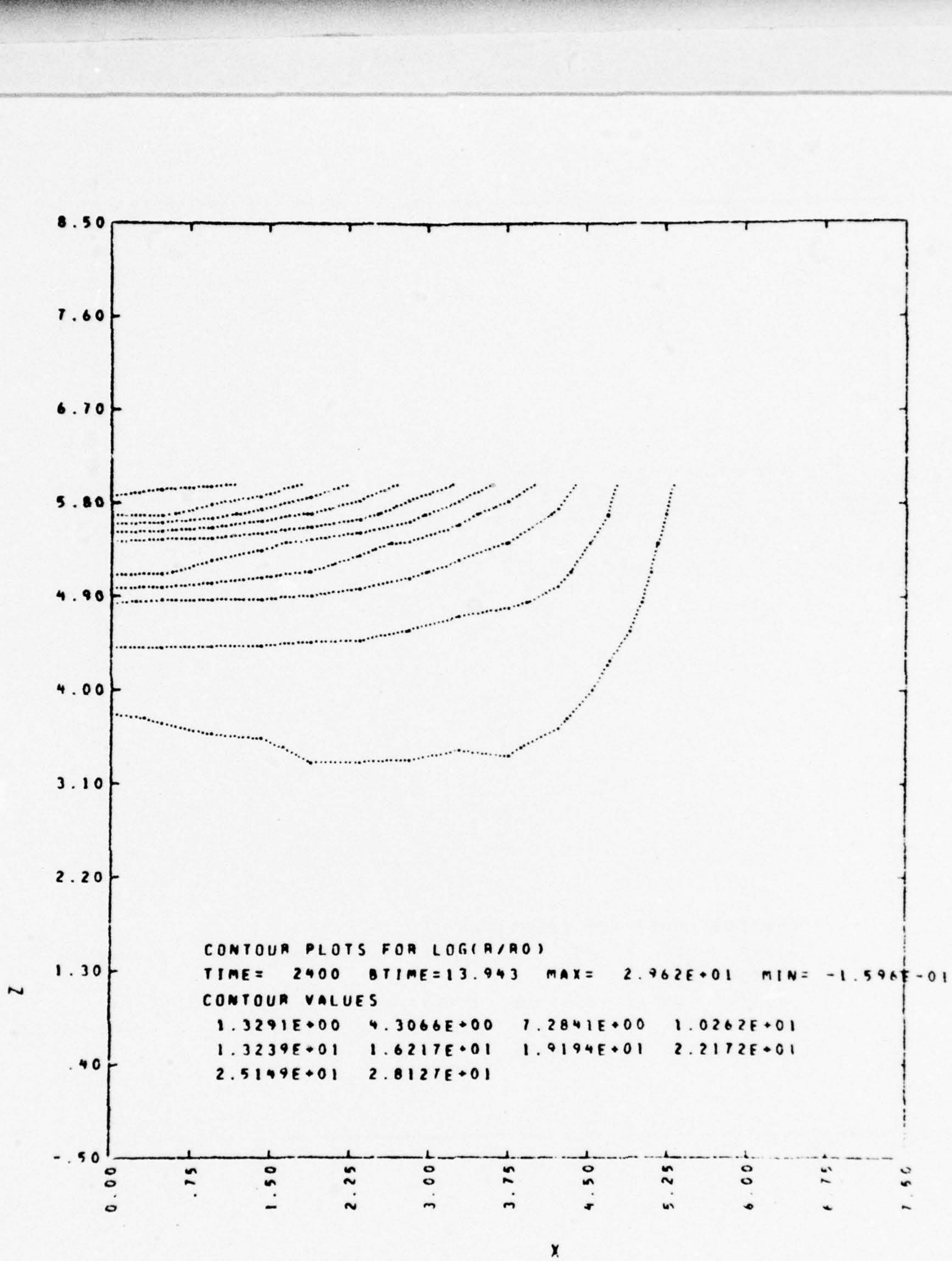

Figure 11. AGW density - 2400 seconds.

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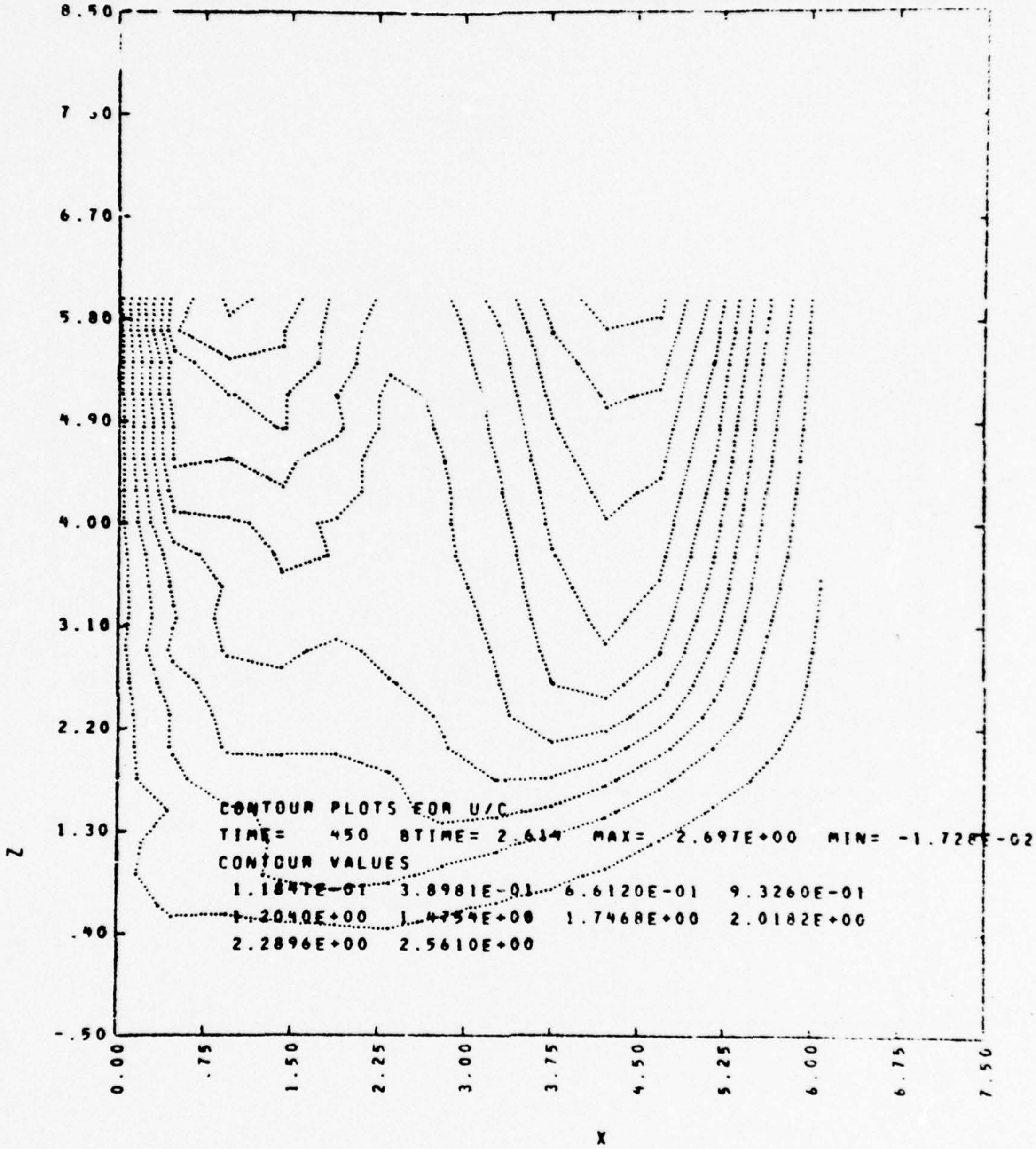

Figure 12. AGW radial velocity - 450 seconds.

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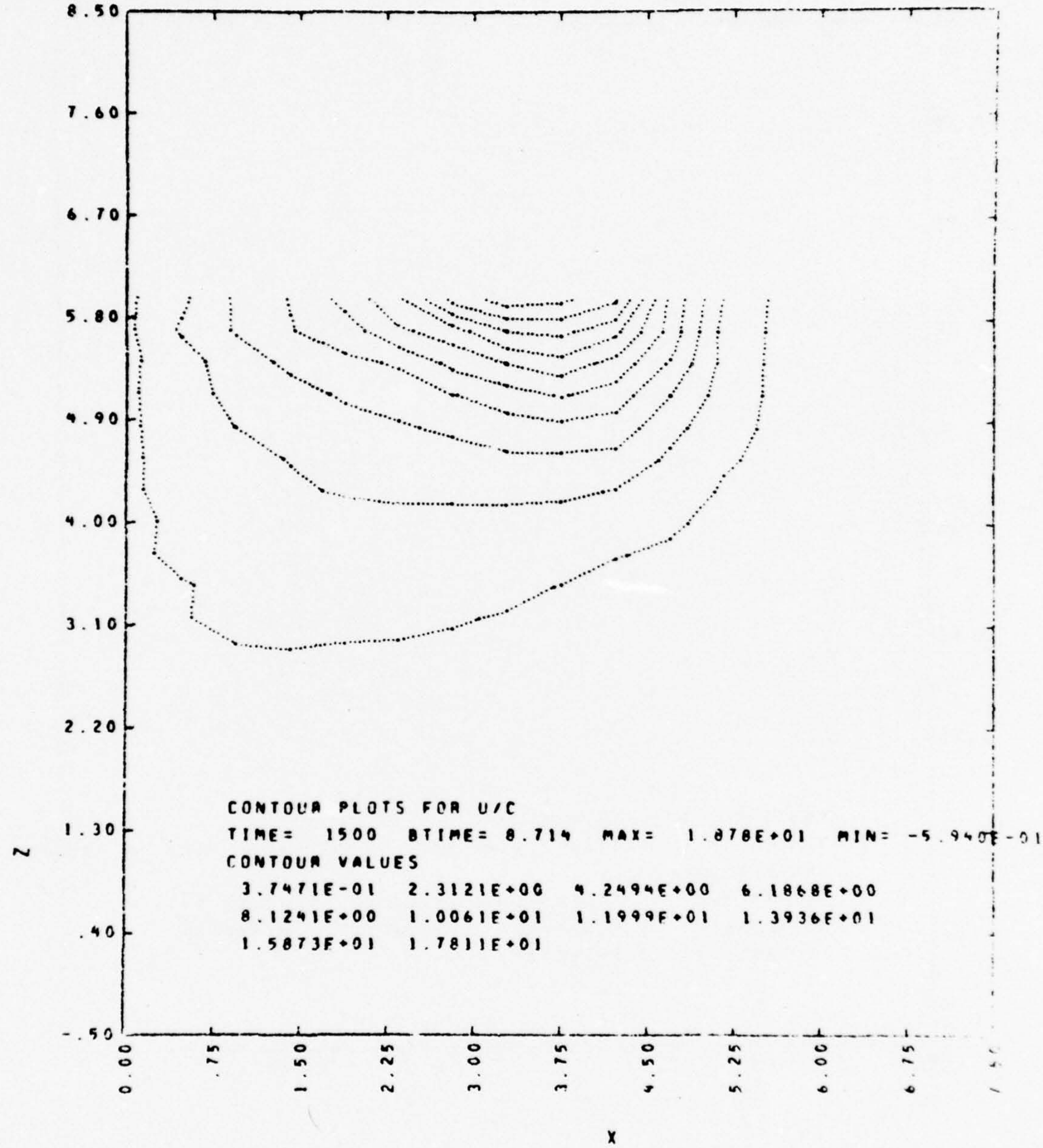

Figure 13. AGW radial velocity - 1500 seconds.

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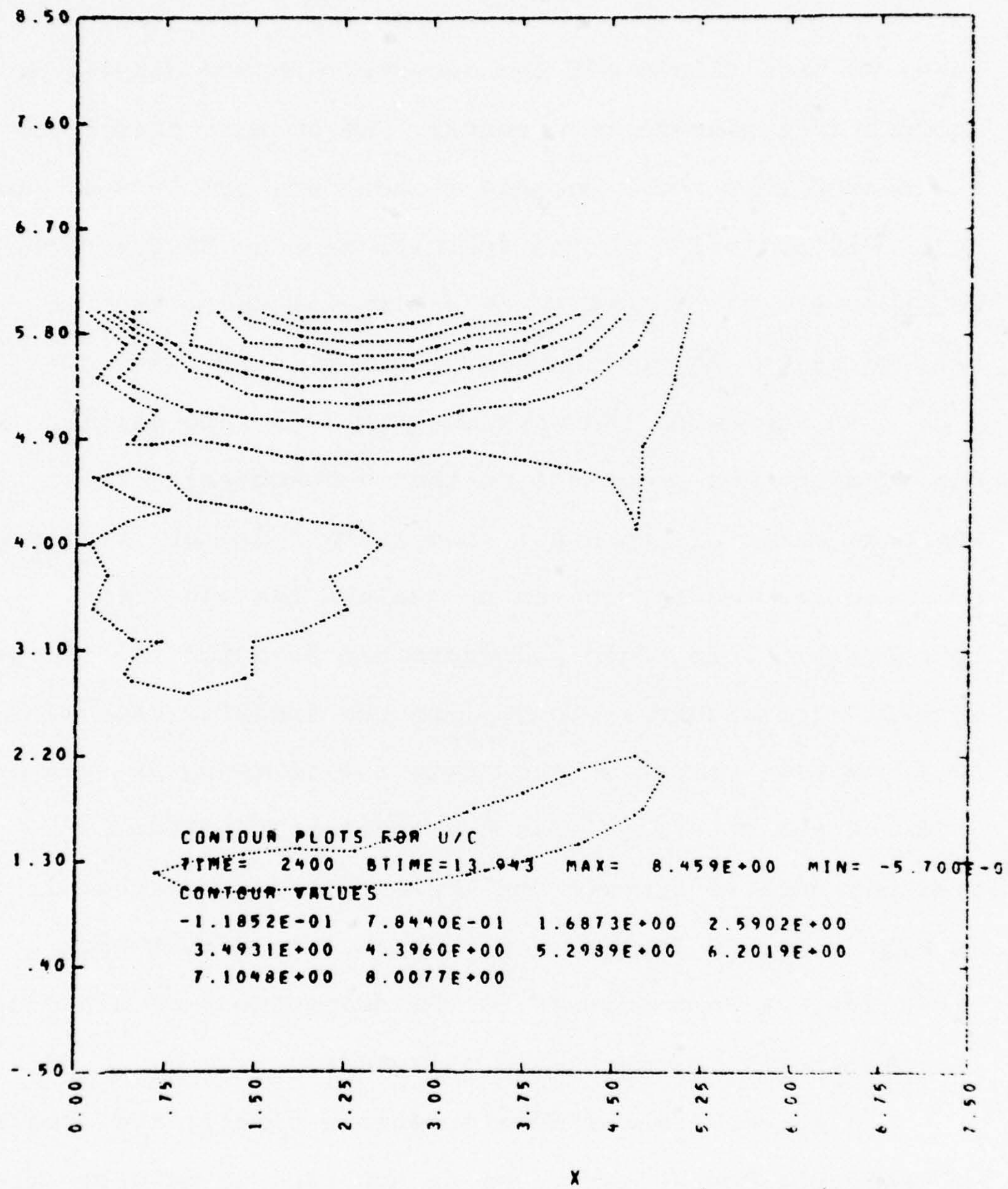

Figure 14. AGW radial velocity - 2400 seconds.

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case, we have sliced off the reservoir in the display to produce an easier-to-read result. We do not attempt to run beyond this point because of boundary problems of our own. Particularly, in the velocity plot at 2400 seconds, we observe what appears to be artificial noise that we believe is coming from boundary reflections.

In reviewing the work described in this section, we can identify two areas for further development. First, it would be desirable to start from hydro code data that does not have large disturbances up against its own grid boundaries. This would eliminate the need for the somewhat wasteful "reservoir region". For the specific case of S200, AFWL is preparing such data for us using an extended grid and the HULL code.[6] As a general proposition, we probably need to pre-process hydro code data so that it is in better format for our application. As a long-term objective, we look forward to the development of convenient "initializers", as mentioned elsewhere.

A second area of development is clearly the problem of "extended boundaries". We do not want to give up our 45 km resolution, but on the other hand, we do not want to increase the mode number above its present value of 131,072. The curious reader may inquire as to why we need so many modes in the first place. Physically, we can

observe that there may only be several hundred "key modes" needed for an excellent fit to a particular data set. Why, then, do we insist on an absolutely "complete set" of all possible modes? The answer is two-fold. In the one case, we want to retain the complete set of acoustic gravity wave physics in order that we can treat arbitrary initial conditions. We will not á priori know the regimes dominated by pressure waves (compression or rarefaction) or by in-running or out-running pure gravity waves. In the second case, we wish to retain a total spatial resolution in order to effectively utilize the FFT. We have explored the concept of incomplete Fourier sets, but these require giving up the FFT. It is important to remember that it is the FFT which permits us to time step this vast mode array in a small fraction of a second on the 7600. We believe that there is an alternative solution to the extended boundary question. This forms the subject of the next section.

III. EXTENDED BOUNDARIES

In previous sections, we have indicated that the use of finite Fourier Transforms imposes distinct boundaries on the AGW modelling effort. We desire to extend these boundaries to very large values. Specifically, there are two related reasons for wishing to extend the overall dimensions of the grid. The first is the problem of running to very late time in the principal battle space itself. If we do nothing, there will arise an apparent "reflection" of waves when the disturbances reach the edge. Created by the periodicity in the finite Fourier Transforms, this effect is unphysical and must be removed. While various "fixes" can and have been imposed in the past, they inevitably introduce an element of noise and uncertainty which grow with time. The ideal solution is, of course, sufficiently extended boundaries to avoid the problem on time scales of interest. The second reason for wishing for more space is the simple desire to generate flow information at more remote locations. Our present data base shows that disturbed wind fields (of interest to striation analysis) extend to the edge of present grids--and thus, logically, beyond.

Obviously, the simple answer to the grid problem is to merely increase its size. Were there no limits to

computer storage this would, of course, be done. The fact is, though, that we already exploit this parameter about as far as practicable. We do not wish to intrude on a major feature of the scheme which empahsizes fast running with no off-line interactive storage. Merely "stretching" the grid, on the other hand, would run the risk of decreasing the resolution below acceptable limits.

It occurred to us some time ago that the inherent characteristics of the FFT-AGW approach ought to allow a sequential, flexible data handling that could get around the problem of large unit storage. It was not, however, unitl the problem was discussed with L.A. Wittwer that a viable scheme was organized.[6] He suggested the concept of analytic interpolation of intermediate modes with storage only of particular reference modes. Instead of a straightforward total FFT of a "big grid", he indicated that it ought to be possible to break the problem into pieces of manageable size by reorganizing the finite Fourier sums. Acting on this intuitively attractive possibility, we have translated the concept into a rational mathematical and numerical routine. An outline of the details is presented as an appendix to this document. We believe that the concept which underlies this approach will have applicability considerably beyond the

particular use that we need for the AGW modelling problem.

We have tested the concept for a relatively simple one-dimensional gravity wave example. The results of this test will be described in the figures which follow. We have begun the task of incorporating the scheme into the full 3-D AGW simulator (the ACCOU code), but the completion of this work lies in the future.

In Figure 15, consider a simple gravity wave in a 32-grid space. As an example, consider each horizontal tick mark to represent 50 km. Figure 16 shows the conventional evolution of the wave in the 1600 km total space. Each vertical display represents the wave amplitude at subsequent time steps. As an example, consider each vertical display to be 100 seconds later than the display above. For the 1 km/sec propagation speed which characterizes this wave packet, we get an apparent reflection at the boundary in 800 seconds. By the time we have progressed to the bottom (2400 seconds), the space is completely muddied up and the physical description bears no relationship to a real unbounded atmosphere.

Figure 17 is the same battle space, but now the effective boundaries have been extended twice as far, equivalent to a 3200 km total space. We display, however, only the original 1600 km space. Now the wave has twice

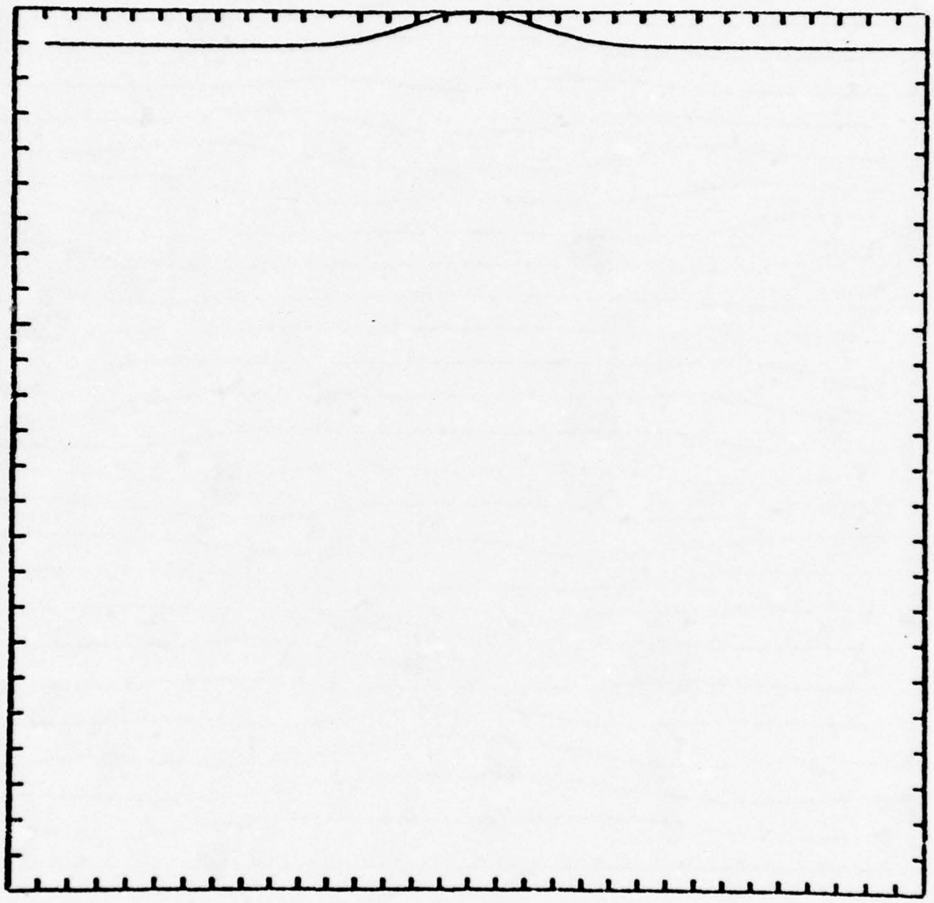

Figure 15. Basic 32 grid - initial wave.

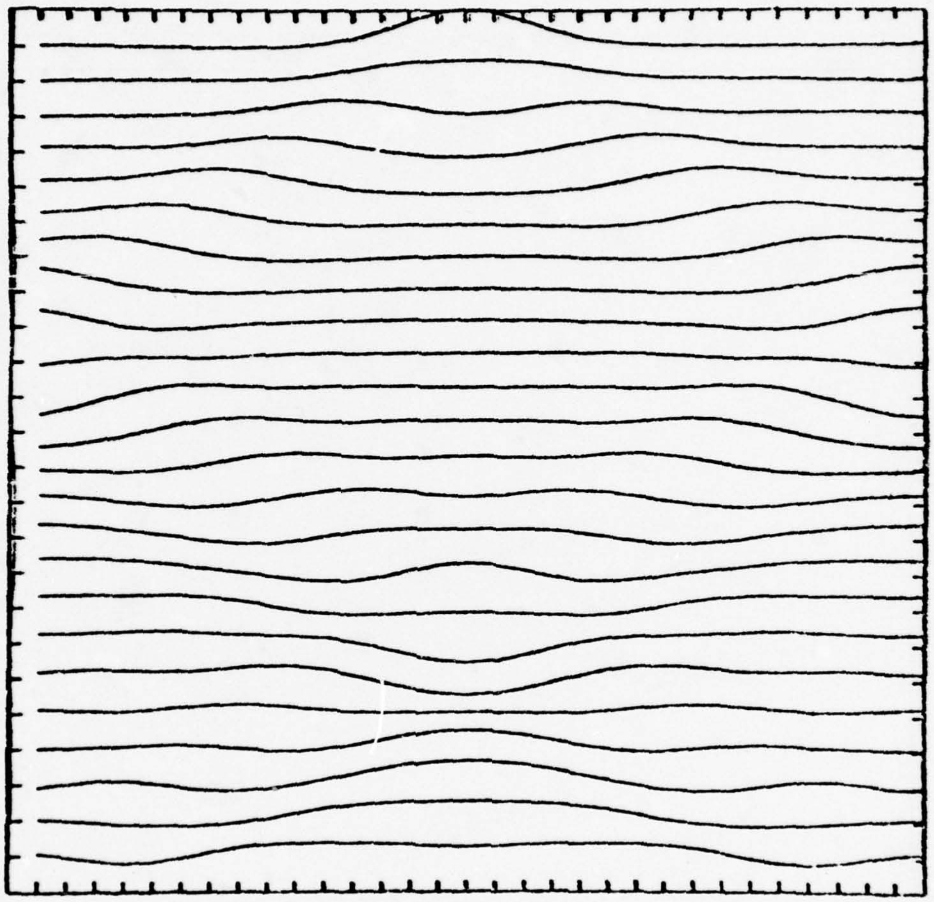

Figure 16. Basic 32 grid - time sequence-1.

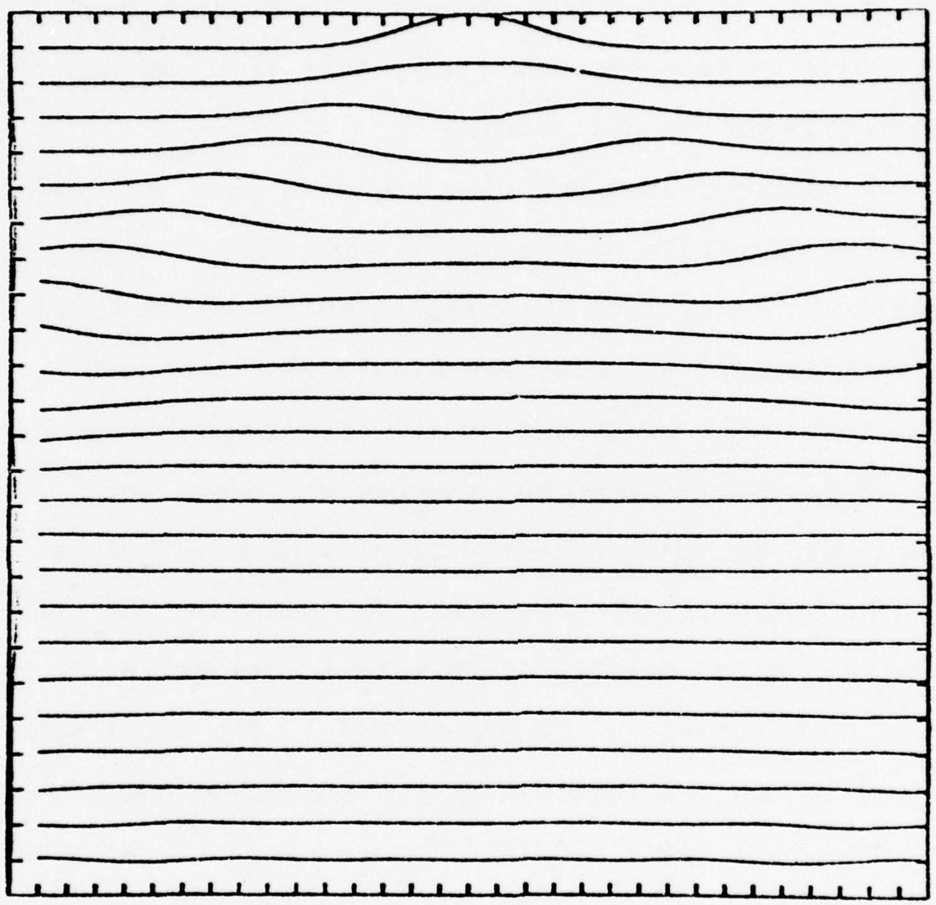

Figure 17. 2x32 grid - time sequence-1.

as far to go and, considering the return time also, will take almost four times as long to be strongly reflected back to the reference grid. Figure 18 continues the scenario out to 4800 seconds and by this time, we see that twice as big is not enough.

In Figure 19, we now play the same game in grand style. The effective boundaries are now made 8 times farther away, equivalent to a 12,800 km space. Nothing comes back in 2400 seconds, and Figure 20 shows that nothing comes back in 4800 seconds. In each of these cases, we have only taken the trouble to return the original 1600 km space with the same 50 km resolution.

In Figure 21, we show the grand scenario for the 8X example. We go for broke and return the entire 256 space using 8 sequential 32-space FFT's. The total space displayed is now the full 12,800 km and we, of course, see why the reflection problem is non-existent. We also see the flexible nature of the scheme which can return the big space at late time when it may be needed.

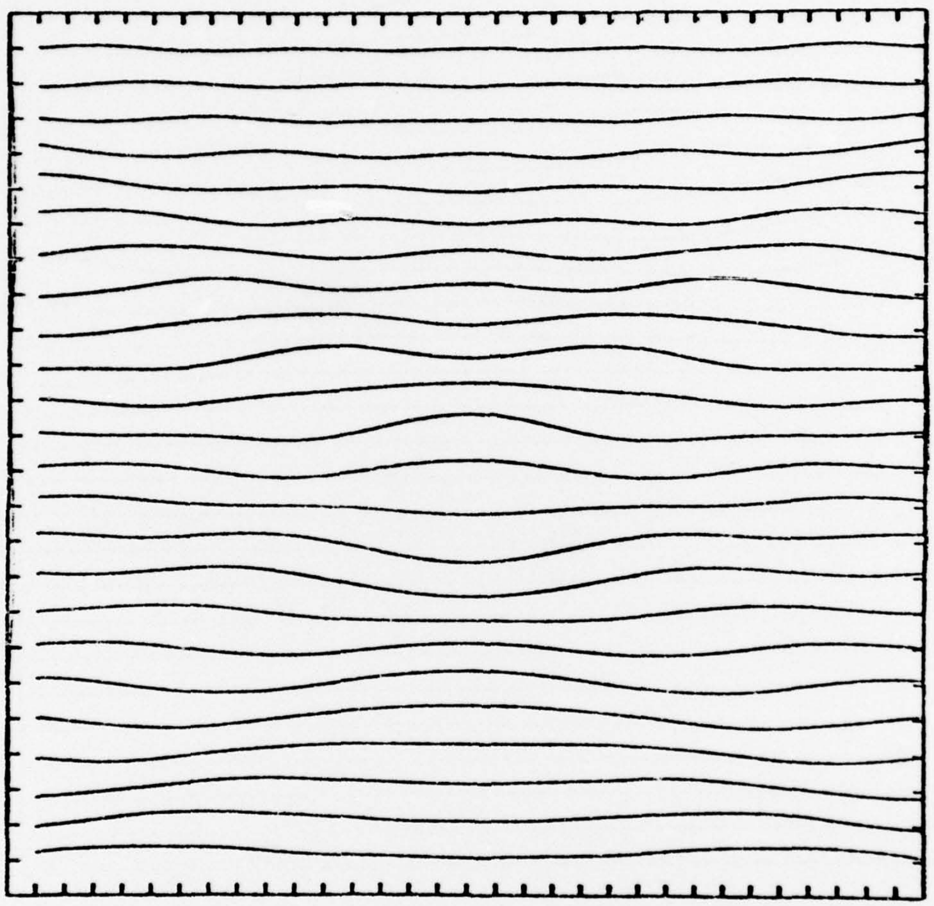

Figure 18. 2x32 grid - time sequence-2.

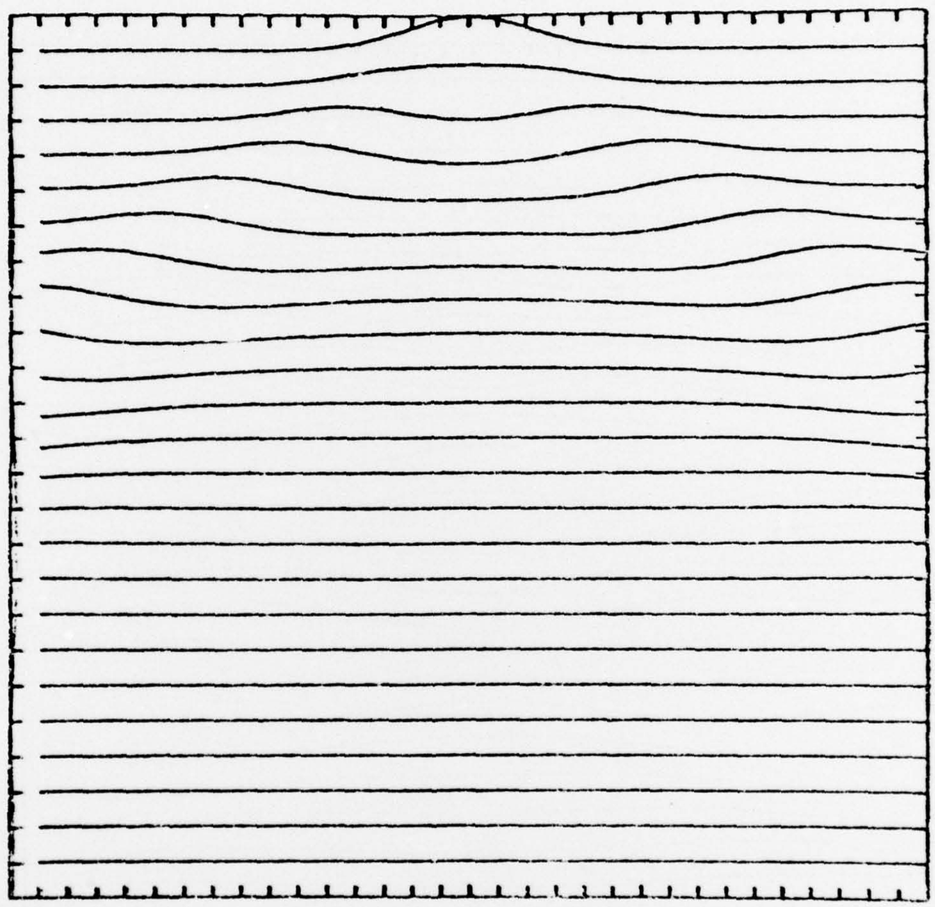

Figure 19. 8x32 grid - time sequence-1.

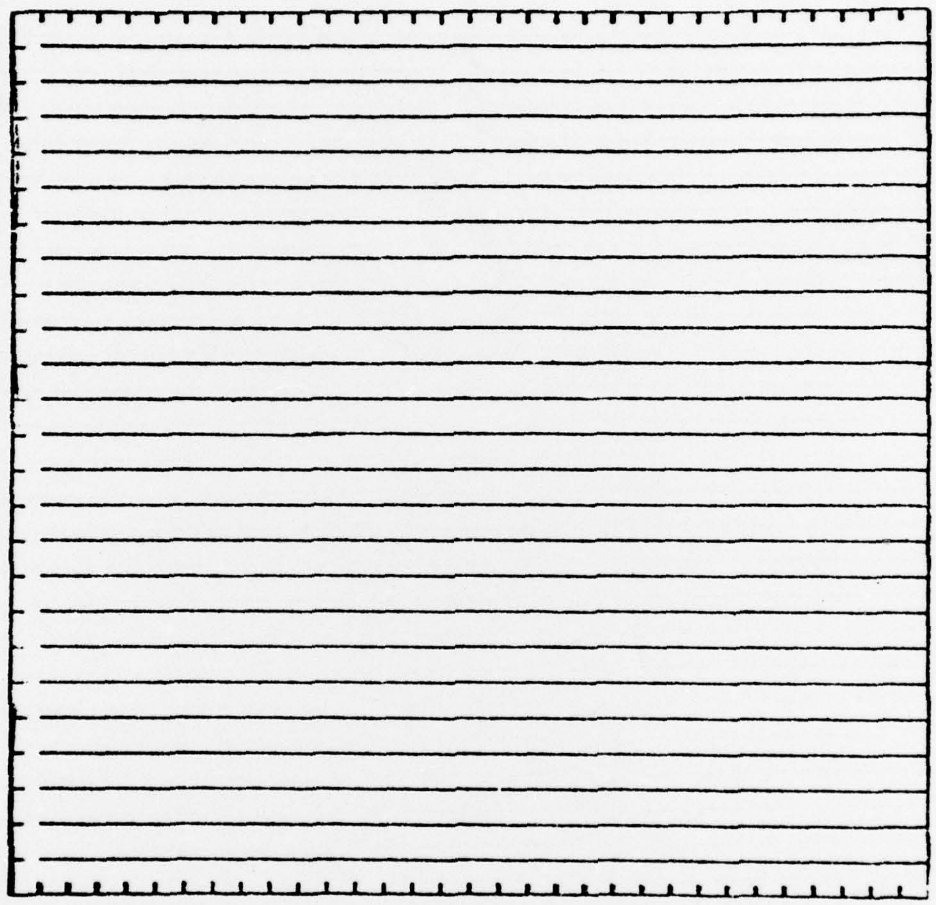

Figure 20. 8x32 grid - time sequence-2.

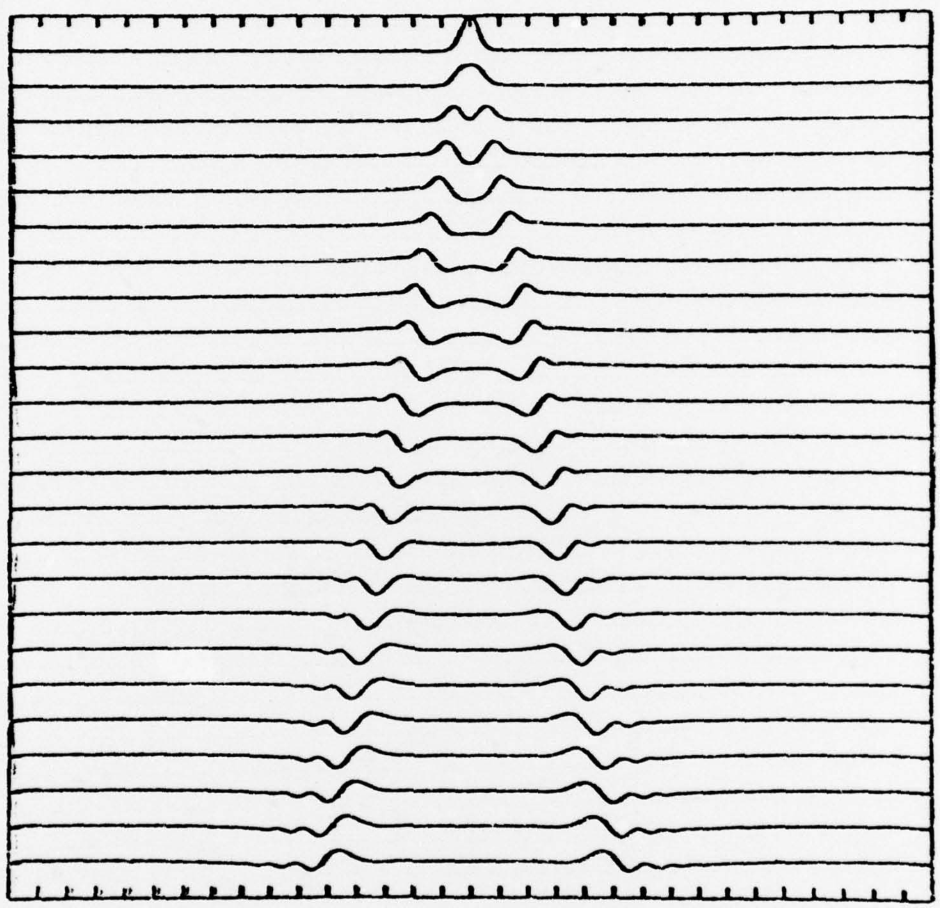

Figure 21. Large 256 grid - time sequence-1.

IV. FUTURE DIRECTIONS

The most important immediate task in AGW model development is the continuation of the effort to incorporate the extended boundary procedure into a full 3-D realization.

On a longer term basis, the question of efficient coupling to general hydro code data will return. In particular, we have not attempted to interface hydro code inputs in multiburst scenarios. Earlier work did, however, display the capability of stopping and restarting with an artificial set of hydro data. We would like to explore the option of starting from a radiation code such as the ROSCOE deposition routine.[2] This capability would provide a wide range of easily accessed initial conditions for parametric studies. Ultimately, we would hope to work closely with any effort to develop a library of flow "initializers".

As the AGW model begins to produce usable output, we will need to explore the interface requirements with a body of plasma phenomenology routines in the community.

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APPENDIX - THE WITTWER-CHU INTERPOLATION SCHEME

For simplicity in discussion and notation, let us describe the interpolation scheme in one dimension. The extension to three dimensions is straightforward but tedious. Consider a finite Fourier Transform of a function, f, which is defined over some interval, L, and is presented as a spatial quantity in the variable, x

$$f(x_s) = \sum_t \hat{f}(k_t)\, e^{ik_t x_s} \tag{A1}$$

The "s" is an index for the space grid of dimension Δx and the "t" is an index for the Fourier grid of dimension Δk.

$$x_s = s\,\Delta x \tag{A2}$$

$$k_t = t\,\Delta k \tag{A3}$$

$$\Delta x = L/N \tag{A4}$$

$$\Delta k = 2\pi/L \tag{A5}$$

$$t,s = 0,\ 1,\ 2 \ldots N-1 \tag{A6}$$

The resolution in physical space is Δx and the solution is periodic (and meaningless) outside of the interval L. The corresponding maximum wavenumber in Fourier space is given by

$$k_{max} = \frac{N\ \Delta k}{2} \tag{A7}$$

and all higher wavenumber modes are assumed not to exist.

If f is a smooth physical variable that we have properly resolved on a grid of dimension Δx, the resolution in Fourier space on dimension Δk will be satisfactory and the function $\hat{f}$ will be smooth in that space.

Because we have a smooth, well resolved function, we would have no trouble interpolating for values of f on dimensions smaller than Δx between grid points in physical space. Likewise, for similar reasons, we will have no trouble interpolating for values of $\hat{f}$ on dimensions smaller than Δk between grid points in Fourier space.

The information obtained by interpolating $\hat{f}$ in Fourier space is exactly the data required to extend the boundary. We can, in fact, extend the boundary as far as we wish, if we are willing to increase our computing time and allow for some additional temporary storage.

Let us assume that we want to extend the boundary (or periodicity) by M times, but, of course, wish to keep Δx fixed. The new grand scale dimension becomes

$$L' = ML \tag{A8}$$

and the corresponding increment in Δk becomes

$$\delta k \equiv (\Delta k)' = \frac{2\pi}{L'} = \frac{1}{M} (\Delta k) \quad . \tag{A9}$$

We can now rewrite our Fourier sum in (A1) as

$$f_n(x_n) = \sum_{t=0}^{N-1} \sum_{\ell=0}^{M-1} \hat{f}(k_t + \ell\delta k) \; e^{ix_n(k_t+\ell\delta k)} \tag{A10}$$

or with a redefinition as

$$f_n(x_n) = \sum_{\ell=0}^{M-1} \left[\sum_{t=0}^{N-1} \hat{g}_\ell \; (k_t) \; e^{ix_n k_t} \right] e^{ix_n \ell\delta k} \tag{A11}$$

where

$$\hat{g}_{\ell=0} \; (k_t) \equiv \hat{f}(k_t) \tag{A12}$$

and

$$\hat{g}_{\ell\neq 0} \; (k_t) \equiv \hat{f} \; (k_t + \ell\delta k) \quad . \tag{A13}$$

We note that the inner sum in (A11) can be expressed as a new, artificial physical space function, g_ℓ ,

$$g_\ell\ (x_n) = \sum_{t=0}^{N-1} \hat{g}_\ell\ (k_t)\ e^{ix_n k_t} \quad . \tag{A14}$$

Thence we can express the grand scale function in (A11) as

$$f_n\ (x_n) = \sum_{\ell=0}^{M-1} g_\ell\ (x_n)\ e^{ix_n \ell \delta k} \tag{A15}$$

At this point, we have assembled all of the basic tools that are required. Let us walk through a computational step to see what actually goes on. Equation (A12) represents the stored array of Fourier data that is always available and which we would have used directly had we not developed the interpolation scheme. Equation (A13) represents Fourier data that is always simply derivable from (A12) by interpolation. It is never permanently stored and is created only when required.

Equation (A14) represents an FFT operation to create the g_ℓ array. Note that it represents an N-dimensional operation. The further step to equation (A15) which creates the real physical variable f is a subsequent FFT

operation on the g_{ℓ} array. Note that it represents an M-dimensional operation.

We would term the above sequence of steps the basic operational mode. We have reconstructed our basic physical variable, f, in the original space of dimension, L. If we were reconstructing f from our array of $\hat{f}$ as a flow variable at "early time", we would presumably see no difference from that of a conventional solution. We would have done more work, however. Instead of a single N-dimensional FFT, we would have required M number of N-dimensional FFT's. We would also have had to temporarily store twice as much data, although the data required in the machine at any moment to perform an FFT was identical.

If, on the other hand, we were reconstructing f from the $\hat{f}$ array at "late time", we would see a dramatic difference in the two cases. The conventional case would have suffered boundary "reflections" and become meaningless. The new case would have proceeded beautifully just as though the boundary associated with L did not exist. It would be functioning in a space equivalent to ML in extent. That is, we would only "see" the data in the interval, L, but the solution would "exist" throughout ML.

Now suppose we had tried to accomplish the above solution by conventional means. We would first have had to

generate and store a permanent $\hat{f}$ array that was M times larger than before. Second, we would have had to bring this data into position all at once to perform an MN-dimensional FFT.

As indicated in an earlier part of the discussion, the effective removal of boundaries in the original battle space interval, L, is not the only purpose of the new procedures. One of our objectives is to obtain flow information at distant locations at late time. To accomplish this task, we employ the same tools, but require one additional step of analysis. A few paragraphs back, when we came to Equation (A10), the careful observer may have noted an apparent change in notation without any mention in the text. The quantities f_n and x_n appeared in place of the expected f and x_s. In the basic mode of operation, these are, in fact, identical quantities. The new indices take on meaning when we consider a reconstruction in the extended domain.

Let us assume that we are interested in reconstructing the flow in some region of our extended space. We desire the information over some interval of dimension L, but not our original interval. We define this space as the "n^{th}" interval (one of a total of M). Our basic physical space grid, x, can be indicated in the new interval by a simple translation

$$x_n = x_s + nL \quad . \tag{A16}$$

Our previous expressions, such as (A14), are periodic in L, thus

$$g_\ell (x_n) = g_\ell (x_s) \quad . \tag{A17}$$

We, thus, can return and use (A15) just as before, but now we employ the new "x_n" in place of the x_s as before. Mathematically, we create a phase change by shifting to the extended value for "x" and then perform the same FFT operation. This step enables us to recover the real physical variable f in an arbitrary interval "n" which was the purpose of the notation f_n.

If we are ambitious, we can reproduce the entire ML space. We do this, however, by reconstructing each part (piece by piece) in sequence. This permits us to develop a massive data bank, if we desire, without increasing our storage requirement on the core of the computer. Obviously, if we want to keep all of this data for subsequent operations, it must be stored outside.

It is by use of the Wittwer-Chu procedures that we hope to maintain 50 km resolution at one point in the simulation and still consider an unbounded space in excess of 12,000 km dimensions.

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